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SIMULATING A MARKOV CHAIN WITH A SUPEREFFICIENT SAMPLING METHOD--ETC(U)

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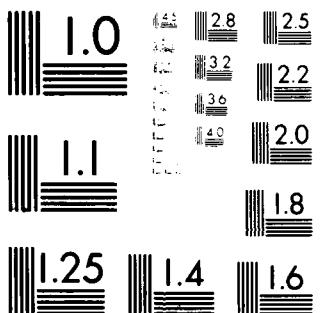
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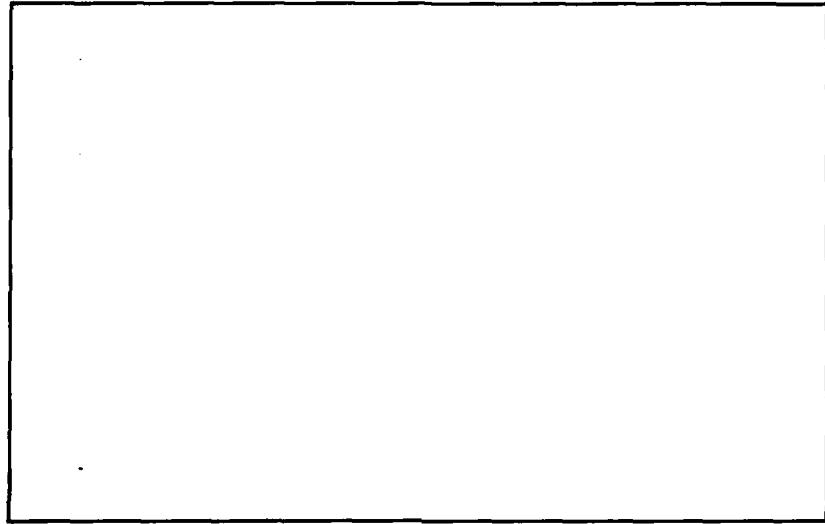
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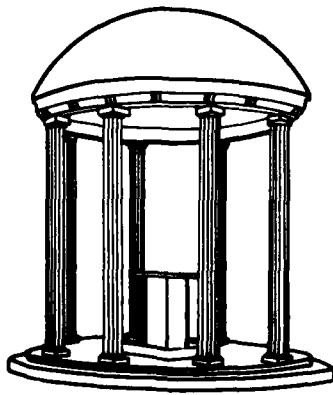
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SIMULATING A MARKOV CHAIN WITH A
SUPEREFFICIENT SAMPLING METHOD

George S. Fishman

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Curriculum in Operations Research
and Systems Analysis
University of North Carolina at Chapel Hill

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Abstract

This paper describes an algorithm and a FORTRAN subprogram, CHAIN, for simulating the behavior of an $(n+1)$ state Markov chain using a variance reducing technique called *rotation sampling*. The simulation of k *microreplications* is carried out in parallel at a mean cost $\leq O(\ln k)$ and with variances of sample quantities of interest $\leq O((\ln k)^2/k^2)$. The program allows for independent *macroreplications*, each of k microreplications, in order to facilitate estimation of the variances of sample quantities of interest. The paper describes theoretical results that underlie the algorithm and program in Section 1 and presents applications of interest for first passage time and steady-state distributions in Section 2. Section 3 describes the algorithm and CHAIN and an example in Section 4 illustrates how CHAIN works in practice. Section 5 describes the options available for restarting the simulation.

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Introduction

A recent paper (Fishman 1981) describes how one can use rotation sampling, a special case of the antithetic variate method, to induce substantial variance reduction in the simulation of a finite state Markov chain. Since many discrete event simulations have an underlying Markov structure or one close to being Markov, this variance reducing proposal has clear appeal. Moreover, for large and possibly ill-conditioned transition matrices, one may prefer the Monte Carlo or simulation method with appropriate variance reducing plans to numerical analysis when solving for steady-state and first passage time distributions. In fact, it may be the only feasible method for some problems.

This earlier work derives its cost-saving potential from viewing the simulation of k tours in *series* of a finite $(n+1)$ state positive recurrent aperiodic Markov chain as equivalent to the simulation of k replications of the Markov chain in *parallel*. Although the marginal distributions that arise with the two alternative formulations are necessarily the same for corresponding variables, the parallel formulation allows one to induce joint distributions across replications that lead to a significant cost saving. The induced joint distributions follow from the use of rotation sampling, as described in detail in Fishman and Huang (1980). The cost saving arises in two ways. Firstly, for fixed n , run time in the correlated case is $O(\ln k)$ in contrast to $O(k)$ for the serial simulation. Secondly, for fixed n the

variance of an estimator of interest has an upper bound $O((\ln k/k)^2)$ for the correlated case compared to $O(1/k)$ for the serial case.

The present paper describes an algorithm for implementing the essential steps for k parallel simulations with correlation along individual sample paths induced by rotation sampling. The paper also describes a FORTRAN program, called CHAIN, that one can use to perform the simulation. In particular, CHAIN runs I independent *macroreplications* each of K correlated parallel *microreplications* and computes point estimates of interest and sample variances of these point estimates.

Section 1 introduces the Markov chain rotation and describes the results on variance reduction derived in Fishman (1981a) for finite state chains. For completeness it also presents results in Fishman (1981b) for infinite state chains. Section 2 describes several potential uses of CHAIN. These include first passage time distributions and steady-state probabilities for semi-Markov processes. Section 3 presents Procedure MC which contains the essential steps in carrying out parallel simulation based on rotation sampling. It also describes the FORTRAN CHAIN subprogram in detail. Section 4 describes an example of how CHAIN can be used in practice. The example is of the discrete time Markov chain that corresponds to the M/M/1 queueing problem with finite capacity n .

1. Definitions and Previous Results

Consider a positive recurrent aperiodic Markov chain with state space $S = \{0, 1, 2, \dots, n\}$ and transition probabilities $\{p_{ij}; i, j = 0, 1, \dots, n\}$

where there exists a positive integer $\delta \leq (n-1)/2$ such that

$$p_{ij} = 0 \quad \text{for } |i-j| > \delta$$

and

(1)

$$\sum_{j=\max(0, i-\delta)}^{i+\delta} p_{ij} = 1$$

It is convenient to describe an alternative, but equivalent, representation to (1) whose value is apparent when actually generating sample paths by simulation on a computer. Let s_j denote the total number of states that have positive transition probabilities from state j and let $\{m_{jr}; r = 1, \dots, s_j\}$ denote the ordered sequence ($m_{jr} < m_{j,r+1}; r = 1, \dots, s_j - 1$) of the s_j states to which entry can occur from state j . Then one has the representation

$$p_{jm_{jr}} > 0 \quad r = 1, \dots, s_j$$

$$\sum_{r=1}^{s_j} p_{jm_{jr}} = 1$$

$$\delta \geq \max (|m_{j1} - j|, |m_{js_j} - j|) \quad j = 0, 1, \dots$$

Suppose one wants to use simulation to study the behavior of the chain during a time period that begins with exit from state a and ends with entry to state $b \in S$. Consider k replications of the simulation experiment run in parallel. Let K'_{ijl} denote the number of replications that move from i to j on transition l and let K'_{jl} be the number of replications in state j at the end of transition l .[†] Let $U, U_1, \dots, U_{K'_{jl}}$ be from $U(0,1)$ where $K'_{jl} > 0$ is given. Then for parallel replications one can represent $K'_{jm_jr^{l+1}}$ as

$$K'_{jm_jr^{l+1}} = \sum_{m=1}^{K'_{jl}} I[q_{j,r-1}, q_{jr})(U_m) \quad (2)$$

where

$$q_{j0} = 0$$

$$q_{jw} = \sum_{r=1}^w p_{jm_jr} \quad w=1, \dots, s_j; j=0, 1, \dots$$

and

$$\begin{aligned} I[u, v)(x) &= 1 & u \leq x < v \\ &= 0 & \text{otherwise.} \end{aligned}$$

To ensure that each replication begins with an exit from state a and ends with the first entry into state b , one replaces

the original $\{p_{bj}; j=1, \dots, s_b\}$ by $p_{bb} = 1$ and sets $p_{bm_{br}} = 0$ for

[†]The prime superscript is used here for consistency with the notation in Fishman (1981a, 1981b). However, without loss of generality, we take the initial state here as a and the final state as b whereas in the earlier work the initial and final states were 0 and a respectively. This relabeling of initial and final states makes the generality of the approach more apparent to the reader.

$r = 1, \dots, s_b$ and $r \neq b$. If $b = a$, these modifications are made after the first transition.

If one uses the *rotation sampling plan*

$$U_m = U + \frac{m-1}{K'_{jl}} \quad 0 \leq U < 1 - \frac{m-1}{K'_{jl}} \quad (3)$$

$$= U + \frac{m-1}{K'_{jl}} - 1 \quad 1 - \frac{m-1}{K'_{jl}} \leq U < 1,$$

then the results in Fishman (1981a,b) apply. In particular,

$$\text{var } K'_{ijl} \leq O(1) \quad (4)$$

and for $S_b = S - b$, the sample number of transitions from i to j is

$$R'_{ijk} = \sum_{l=1}^{\infty} K'_{ijl} \quad (5a)$$

and the sample mean reward is

$$R'_k = \frac{1}{k} \sum_{l=1}^{\infty} \sum_{i \in S_b} \sum_{j \in S} A_{ij} K'_{ijl} . \quad (5b)$$

Then one has

$$\text{var } R'_{ijk} \leq O((\ln k)^2) \quad (5c)$$

and, if $|A_{ij}| \leq O(1)$,

$$k^2 \text{var } R'_k \leq O(\delta^2 (\ln k)^4) \quad \text{as } n \rightarrow \infty \quad (5d)$$

$$k^2 \text{var } R'_k \leq O((n\delta \ln k)^2) \quad n < \infty.$$

Here we speak of $\{A_{ij}\}$ as the reward function. Finally, the number of steps to total absorption

$$T'_k = \min(t: K'_{bt} = k)$$

has

$$E T'_k = O(\ln k) \quad (6)$$

and

$$\text{var } T'_k \leq O((\ln k)^2).$$

Note that the sampling scheme (3), when used in (2), preserves the identical and correct probability laws along the sample paths of each of the k replications. An equivalent expression for $K'_{jm_{jr}^{l+1}}$, which leads to a computational saving, is:

$$\begin{aligned} K'_{jm_{jr}^{l+1}} &= |Q| - |P| + I_{[\bar{P}, \bar{Q}]}(\overline{K'_{j\ell} U}) \quad \bar{P} \leq \bar{Q} \\ &= |Q| - |P| - I_{[\bar{Q}, \bar{P}]}(\overline{K'_{j\ell} U}) \quad \bar{P} > \bar{Q} \end{aligned} \quad (7)$$

where

$$P = K'_{j\ell} q_{j,r-1},$$

$$Q = K'_{j\ell} q_{jr}$$

and $\bar{x} = x - \lfloor x \rfloor$. Here the cost of sampling the transitions from state j based on (7), and using the inverse transform method, is $O(s_j) \leq O(2\delta + 1)$ and independent of k whereas sampling cost based on (2) is at best $O(k)$.

Let S'_k denote the cost of simulating (1) using (3) in (7). For a countably infinite state space, no more than $(2\delta + 1)\ell$ transient states are occupied prior to transition $\ell+1$ and, therefore, no more than $(2\delta + 1)(\ell^2 + \ell)/2$ sampling events occur through transition ℓ . Since each (i,j) transition has cost $O(2\delta + 1)$, one has $S'_k \leq O((\delta T'_k)^2)$ so that

$$E S'_k \leq O((\delta \ln k)^2). \quad (8a)$$

For the finite state case

$$E S'_k \leq O(n \delta \ln k). \quad (8b)$$

These results compare favorably with the case of independent replications taken in series where R_{ijk} and R_k , the sample number of transitions from i to j and the sample mean reward, respectively, have $\text{var } R_{ijk} = O(k)$ and $k \text{ var } R_k = O(1)$. Moreover, for simulation cost S_k , one has $O(k) \leq E S_k \leq O(\delta k)$. The lower bound arises when n is small enough to allow storage of all distributions and their aliases required by the alias method (Walker 1977) to determine the entered state from each existing state at each transition. The upper bound arises from use of the inverse transform method to determine the paths. See Fishman (1981b) for a more detailed discussion of this cost.

It is also noteworthy that the desirability of k parallel replications with rotation sampling relative to a simulation of k independent replications in series continues to hold when $\{A_{ij}\}$ is not bounded, provided that $\text{var}(A_{ij} | K'_{ij,\ell+1} | K'_{il}) < \infty$.

2. Potential Uses

This section describes three uses to which the previously described rotation sampling plan can be put with regard to estimation.

First Passage Times

Let

h_ℓ = probability of moving from state a to state b for the first time in exactly ℓ steps

and

$H_\ell = \sum_{i=1}^{\ell} h_i$ = probability of moving from state a to state b for the first time in no more than ℓ steps.

(9)

As estimators of h_ℓ and H_ℓ one has, respectively,

$$\hat{h}_\ell = \frac{1}{k} \sum_{j \in S_b} K'_{jb\ell} = \frac{1}{k} (K'_{b\ell} - K'_{b,\ell-1}) \quad K'_{b0} = 0$$

and

$$\hat{H}_\ell = \frac{1}{k} \sum_{i=1}^{\ell} \sum_{j \in S_b} K'_{jbi} \quad \ell = 1, 2, \dots$$

(10)

Let $S'_{k\ell}$ denote the cost of simulating (1) up to and including step using the rotation sampling plan (3) with (7). Theorem 1 gives several relevant properties for \hat{h}_ℓ , \hat{H}_ℓ and $S'_{k\ell}$.

Theorem 1. For a simulation of k parallel replications of (1) using (3) and (7) one has:

- (i) $E \hat{h}_\ell = h_\ell$.
- (ii) $E \hat{H}_\ell = H_\ell$.
- (iii) $\text{var } \hat{h}_\ell \leq O((\delta/k)^2)$.
- (iv) $\text{var } \hat{H}_\ell \leq O((\delta\ell/k)^2)$.
- (v) $E S'_{k\ell} \leq O((\delta\ell)^2)$.

Proof. Since the correct probability law continues to prevail on sample paths for each replication, one has $E K'_{jbl} = k h_\ell$ so that (i) and (ii) follow immediately. Since $\text{var } K'_{jbl} \leq O(1)$ and no more than 2δ states can transit to state b , it is clear that

$$\text{var}(\sum_{j \in S_b} K'_{jbl}) \leq O(\delta^2)$$

and that (iii) holds. Since there are exactly ℓ steps to consider, (iv) follows immediately. Here \hat{H}_ℓ is a special case of (5b) with $A_{ib} = 1$ if $i \in S_b$ and $A_{ij} = 0$ otherwise. Since exactly ℓ steps occur no more than $(2\delta + 1)(\ell^2 + \ell)/2$ trials are necessary each with cost $O(\delta)$. Therefore, (v) obtains.

If one were to perform k independent replications in series, then $\text{var } \hat{h}_\ell = O(1/k)$, $\text{var } \hat{H}_\ell = O(\ell^2/k)$ and $E S_k \geq O(k)$, emphasizing the benefit of rotation sampling plan (3) and the conciseness of (7).

Steady-State Distribution

Let

p_j = probability of being in state j at an arbitrarily selected time $j = 0, 1, \dots, n$.

As an estimator of p_j one has

$$\hat{p}_j = G_{jk}/G_k \quad (11)$$

where

$$G_{jk} = \frac{1}{k} \sum_{t=1}^{\infty} \sum_{i=0}^n K'_{ijt} \quad j=0, 1, \dots, n$$

and

$$G_k = \sum_{j=0}^n G_{jk}.$$

Since \hat{p}_j is a *ratio* estimator it has bias

$$E(\hat{p}_j - p_j) \doteq p_j^2 \left[\frac{\text{var } G_k}{E^2 G_k} - \frac{\text{cov}(G_{jk}, G_k)}{E G_{jk} \cdot E G_k} \right] \quad (13)$$

and variance

$$\text{var } \hat{p}_j \doteq p_j^2 \left[\frac{\text{var } G_k}{E^2 G_k} - \frac{2 \text{cov}(G_{jk}, G_k)}{E G_{jk} \cdot E G_k} + \frac{\text{var } G_{jk}}{E^2 G_{jk}} \right]. \quad (14)$$

From the results of Section 1, one has

$$\text{var } G_{jk} \leq O((\delta \ln k/k)^2) \quad \text{and} \quad \text{var } G_k \leq O((n \ln k/k)^2)$$

so that both bias and variance benefit from rotation sampling.

Steady-State Probabilities for a Semi-Markov Process

The results presented so far relate directly to a Markov chain. However, their extension to semi-Markov processes is relatively direct for the steady-state probabilities. Let μ_{ij} denote the mean time spent in state i prior to transiting to state j . For the steady-state probabilities, one now has the estimators

$$\tilde{p}_j = G'_{jk}/G'_k \quad j=0, \dots, n$$

where

$$G'_{jk} = \sum_{t=1}^{\infty} \sum_{i=0}^n \mu_{ij} K'_{ijt}$$

and

$$G'_k = \sum_{j=0}^n G'_{jk} .$$

Then \tilde{p}_j has approximate bias and variance as in (13) and (14), respectively, with G'_{jk} replacing G_{jk} and G'_k replacing G_k .

3. Implementation

Procedure MC describes an algorithm that one can use to encode the essential steps for simulating k replications in parallel with initial state a and absorbing state b . In practice, one will want to embellish this procedure to allow for multiple reward functions and multiple independent macroreplications. The latter enable one to estimate variances and covariances of interest.

Figure 1 lists a FORTRAN subprogram called CHAIN that enables one to simulate an $(N + 1)$ state Markov chain with state space on the integers $0, 1, \dots, N$ using the parallel rotation sampling plan (7) for the purpose of computing sample mean rewards $RPRIME(1), \dots, RPRIME(L)$ for L reward matrices stored in array $A(\cdot)$. Each of I independent *macroreplications* begins with a departure of K correlated *microreplications* from state INITIAL and ends with the absorption of all K microreplications in state ABSORB. The purpose of the macroreplications is to facilitate the estimation of the covariance matrix of the L sample mean reward functions. Also, CHAIN estimates the first passage time distribution from INITIAL to ABSORB.

Insert Fig. 1 about here.

Procedure MC

Given: $a, b, k, n, \{s_i; i=0, \dots, n\}, \{m_{ir}; r=1, \dots, s_i; i=0, \dots, n\},$
 $\{p_{i,m_{ir}}; r=1, \dots, s_i; i=0, \dots, n\}$ and $\{A_{im_{ir}}; r=1, \dots, s_i, i = 0, \dots, n\}.$

1. $i \leftarrow a.$
 2. $R' \leftarrow 0.$
 3. $K'_a \leftarrow k.$
 4. For $i=0, \dots, n$
 For $r=1, \dots, s_i$

$$q_{i,m_{ir}} \leftarrow \sum_{l=1}^{s_i} p_{i,m_{il}}.$$

 $K_i^* \leftarrow 0.$
5. Go to 8.
 6. $i \leftarrow 0.$
 7. If $i=b$ or $K'_i = 0$ go to 23. (Skip if state is absorbing or empty.)
 8. $r \leftarrow 1.$
 9. Sample U from $U(0,1).$
 10. $P^* \leftarrow 0.$
 11. $\bar{P} \leftarrow 0.$
 12. $Q \leftarrow K'_i q_{i,m_{ir}}.$
 13. $Q^* \leftarrow \lfloor Q \rfloor.$
 14. $\bar{Q} \leftarrow Q - Q^*.$
 15. $X \leftarrow Q^* - P^* + \frac{1}{2} [\text{sign}(U-\bar{P}) + \text{sign}(\bar{Q}-U)].$
 16. $K_{m_{ir}}^* \leftarrow K_{m_{ir}}^* + X.$ (X microreplications move from i to $m_{ir}.$)
 17. $R' \leftarrow R' + X A_{i,m_{ir}}.$ (Compute reward.)
 18. $P^* \leftarrow Q^*.$
 19. $\bar{P} \leftarrow \bar{Q}.$
- } Initialize.
- } Rotation Sampling

20. If $i=b$, $K'_b \leftarrow 0$. (In case $a = b$.)
21. $r \leftarrow r + 1$.
22. If $r \leq s_i$ go to 12.
23. $i \leftarrow i + 1$.
24. If $i \leq n$ go to 7.
25. $i \leftarrow 0$.
26. If $i=b$ go to 33.
27. $r \leftarrow 1$.
28. If $m_{ir} = b$, $K'_b \leftarrow K'_b + K^*_b$ and go to 30. (Arrange for absorptions.)
29. $K'_{m_{ir}} \leftarrow K^*_{m_{ir}}$. (Move to transient states.)
30. $K^*_{m_{ir}} \leftarrow 0$.
31. $r \leftarrow r + 1$.
32. If $r \leq s_i$ go to 28. (Are all moves from i completed?)
33. $i \leftarrow i + 1$.
34. If $i \leq n$ go to 26.
35. If $K'_b < k$ go to 6. (Are all absorbed?)
36. $R' \leftarrow R'/k$ and deliver R' .

Figure 2 contains a partitioned list of the input to CHAIN. Figure 2a displays all arrays and variables for which an initial numerical assignment is necessary at the time at which CHAIN is called. Figure 2b contains all interim working arrays and Fig. 2c lists all output arrays.

Insert Fig. 2 about here.

Note that the arrays A, M and P are one-dimensional in the subprogram whereas their counterparts $\{A_{ij}\}$, $\{m_{ij}\}$ and $\{p_{ij}\}$ are doubly subscripted in Section 1. This reduction leads to a considerable space saving, especially when $\{A_{ij}\}$, $\{m_{ij}\}$ and $\{p_{ij}\}$ are sparse and N is large. In terms of storage space, CHAIN requires $O(4(\text{ALL}(L+4) + 2L(L+3) + 4NP + \text{SIZE} + 8TT))$ bytes for the arrays listed in Fig. 2. Also, CHAIN has an upper bound on mean execution time of $O(\text{ALL} \times I \times L \times \ln K)$.

CHAIN uses the GGUBS random number generator in IMSL (1977) with SEED as the seed or initial random number and returns SIZE uniform deviates on each call of the generator. By choosing the blocking factor SIZE to be large one reduces the frequency of calling GGUBS, thus reducing CPU time. However, the space requirement for the uniform deviates is $4 * \text{SIZE}$ bytes. On a computer with limited space, one may select a small SIZE to accomodate the space constraint. More generally, an alternative random number generator can be substituted by GGUBS with little effort.

The input OLD also calls for explanation. After running CHAIN for, say I_1 independent macroreplications each of K correlated microreplications, a user may find that the accuracy of the sample mean rewards is too low for intended purposes. By setting OLD = I_1 on a second run,

choosing a new $I > OLD$, using the original K and restoring $XBAR(*)$ and $COV(*,*)$ in the *driver program*, one can merge the sample output from the first OLD macroreplications with that from the subsequent $I - OLD$ new macroreplications to produce a summary tableau. When this is done, the resulting sample first passage time distribution is based on the last $I - OLD$ macroreplications only.

Macroreplication versus Microreplication

As Section 1 shows, rotation sampling applied to K parallel microreplications produces a covariance matrix whose convergence rate has an upper bound $O((\ln K)^2/K^2)$ on a single macroreplication. Since a method is not yet available for estimating this covariance matrix from a single macroreplication, CHAIN resorts to running I independent macroreplications for the purpose of estimating the covariance matrix of the L sample reward functions. Therefore, the covariance matrix has a convergence rate bounded by $O((\ln K)^2 / IK^2)$ and a run time of $O(I \ln K)$ for fixed ALL and L . Clearly one wants a K substantially larger than I . In the example to be described next $K = 2^{17}$ and $I = 2^3$, but other compromises are equally reasonable.

4. An Example

To illustrate how the CHAIN subprogram works in practice, consider the Markov chain associated with the M/M/1 queueing problem with finite capacity n . In particular, the state of the chain denotes the number

of customers in the system. In this queueing problem interarrival times are i.i.d. from the exponential distribution with rate λ , service times are i.i.d. from the exponential distribution with rate $\omega > \lambda$ and there is a single server. For the corresponding Markov chain these specifications imply

$$p_{01} = 1$$

$$p_{i,i-1} = \frac{\omega}{\lambda+\omega} \quad i=1, \dots, n$$

$$p_{i,i+1} = \frac{\lambda}{\lambda+\omega} \quad i=1, \dots, n-1$$

$$p_{n,n} = \frac{\lambda}{\lambda+\omega}$$

with all other transition probabilities being zero.

As objectives consider the estimation of

W_1 = mean number in system.

W_2 = probability of one customer in the system.

W_3 = probability of two customers in the system.

W_4 = first passage time probability mass function for the Markov chain from the empty and idle state back to that state.

W_5 = distribution function associated with W_4 .

Let $\{A_{ij}(\ell)\}$ denote reward matrix ℓ and $R'_k(\ell)$ denote sample mean reward function ℓ based on using $\{A_{ij}(\ell)\}$ in (5b). Then one estimates W_1 , W_2 and W_3 by

$$\hat{W}_1 = R'_k(1)/R'_k(2)$$

$$\hat{W}_2 = R'_k(3)/R'_k(2)$$

$$\hat{W}_3 = R'_k(4)/R'_k(2)$$

where

$$A_{i,i+1}(1) = \frac{i+1}{\lambda+\omega} \quad i=0, \dots, n-1$$

$$A_{i,i-1}(1) = \frac{i-1}{\lambda+\omega} \quad i=1, \dots, n$$

$$A_{n,n}(1) = \frac{n}{\lambda+\omega}$$

$$A_{10}(2) = \frac{1}{\lambda}$$

$$A_{i,i+1}(2) = \frac{1}{\lambda+\omega} \quad i=0, \dots, n-1$$

$$A_{i,i-1}(2) = \frac{1}{\lambda+\omega} \quad i=2, \dots, n$$

$$A_{n,n}(2) = \frac{1}{\lambda+\omega}$$

$$A_{10}(3) = \frac{\omega}{\lambda+\omega}$$

$$A_{12}(3) = \frac{\lambda}{\lambda+\omega}$$

$$A_{21}(4) = \frac{\omega}{\lambda+\omega}$$

$$A_{23}(4) = \frac{\lambda}{\lambda+\omega} .$$

For W_4 and W_5 we use the estimators in (10). These are computed automatically by CHAIN.

Figure 3 shows a driver program designed to initialize all relevant

parameters and call CHAIN for this problem. Here LAM and W correspond to λ and ω

Insert Fig. 3 about here.

respectively. As input we set

LAM = 0.9

W = 1.0

N = 49

INITAL = 0

ABSORB = 0

I = $2^3 = 8$

K = $2^{17} = 131072$

L = 4

SEED = 1234567

SIZE = 40000

TT = 50 .

Figure 4 shows the output of CHAIN for this problem. The ratio estimators W_1 , W_2 and W_3 together with their biases and variances can

Insert Fig. 4 about here.

be computed by hand or by a subsequent subroutine that uses XBAR and COV as input together with the formulae

$$E\left(\frac{Y}{X} - \frac{EX}{EX}\right) \doteq \frac{EY}{EX} \left[\frac{\text{var } X}{E^2 X} - \frac{\text{cov}(X, Y)}{EX \cdot EY} \right]$$

and

$$\text{var}\left(\frac{Y}{X}\right) \doteq \frac{E^2 Y}{E^2 X} \left[\frac{\text{var } X}{E^2 X} - \frac{2 \text{cov}(X, Y)}{EX \cdot EY} + \frac{\text{var } Y}{E^2 Y} \right] .$$

We have chosen to do them by hand. They are

$$\begin{aligned} \hat{W}_1 &= 8.7396 & \hat{W}_2 &= .0905 & \hat{W}_3 &= .0814 \\ E(\hat{W}_1 - W_1) &\doteq -.1037 \times 10^{-4} & E(\hat{W}_2 - W_2) &\doteq .4304 \times 10^{-7} & E(\hat{W}_3 - W_3) &\doteq .3735 \times 10^{-7} \\ \text{var } \hat{W}_1 &\doteq .2646 \times 10^{-3} & \text{var } \hat{W}_2 &\doteq .3780 \times 10^{-8} & \text{var } \hat{W}_3 &\doteq .2936 \times 10^{-8} . \end{aligned}$$

From Gross and Harris (1974, Sec. 2.5) one has

$$W_1 = 8.7410 \quad W_2 = .0905 \quad W_3 = .0814 ,$$

which confirm the performance of CHAIN.

All computing was performed on an IBM 370/155 computer. For FORTRAN G (level 21), the CHAIN Program requires 8592 bytes of space. For FORTRAN H (level 21.8) it requires 7380 bytes.

5. Restarting the Simulation

Situations will occur in which a user of CHAIN does not have a good a priori estimate of the running time or the statistical reliability to be expected from a specified set of I_1 macroreplications each of K_1 microreplications. At least two alternatives exist for dealing with this case. A user may make a preliminary run and determine that I_2 additional macroreplications, each of $K_2 = K_1$ microreplications, are necessary to achieve the desired accuracy within budget. CHAIN is designed to accommodate this alternative and, provided that the sample means and covariances accumulated on the first I_1 macroreplications are restored prior to collecting the additional I_2 macroreplications, the routine prints the global sample means and covariances at the end of all $I_1 + I_2$ macroreplications.

The second alternative arises when on the basis of the first run a user determines that I_2 macroreplications each of $K_2 \neq K_1$ microreplications is the most desirable way of achieving the desired accuracy. Here the restoration feature of CHAIN does not apply. Let \bar{X} and Σ be the sample mean vector and sample covariance matrix of \bar{X} obtained on the first run with I_1 and K_1 . Let \bar{Y} and Ω denote the corresponding quantities on the second run with I_2 and K_2 . Then the overall sample mean vector is

$$\bar{Z} = \frac{1}{(I_1 + I_2)} (I_1 \bar{X} + I_2 \bar{Y})$$

and its sample covariance matrix is

$$\bar{\Gamma} = \frac{1}{(I_1 + I_2)^2} (I_1^2 \Sigma + I_2^2 \Omega) .$$

Although the computation of \bar{Z} and \bar{I} are not features of CHAIN one can easily add them if desired. However, as in the case of the ratio estimators in Section 4, the relative importance of this feature will differ from user to user.

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```

SUBROUTINE CHAIN(K,OLD,I,NP,INITAL,ABSORB,S,M,SUMS,ALL,P,
1      KPRIME,KSTAR,Q,L,ASIZE,A,RPRIME,XBAR,COV,COEFF,
2      TT,PRBAR,PRVAR,CUMBAR,CUMVAR,SEED,SIZE,V)          00000100
C *** PROGRAM FOR SIMULATION OF MARKOV CHAIN WITH M+1 STATES 00000110
C *** USING ROTATION SAMPLING.                                00000120
00000130
00000140
00000150
00000160
00000170
00000180
00000190
00000200
00000210
00000220
00000230
00000240
00000250
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000330
00000340
00000350
00000360
00000370
00000380
00000390
00000400
00000410
00000420
00000430
00000440
00000450
00000460
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00000500
00000510
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00000560
00000570
00000580
00000590

C *** DESCRIPTION OF VARIABLES -
C ***
C *** A(*)      = REWARD MATRIX
C *** ABSORB    = ABSORBING STATE
C *** ALL        = SUM OF S(J) FOR ALL J
C *** ASIZE     = SIZE OF A ARRAY
C *** B          = TEST VARIABLE
C *** C          = ((LI-1)/LI)
C *** CC         = ((LI-OLD-1)/(LI-OLD))
C *** COEFF(*)  = COEFFICIENTS OF VARIATION
C *** COUNT     = UNIFORM DEVIATE COUNTER
C *** COV(*,*)   = COVARIANCE MATRIX
C *** CUM        = ACCUMULATION OF FREQ
C *** CUMDAR(*) = MEAN OF CUM
C *** CUMCV     = COEFFICIENT OF VARIATION FOR CUM
C *** CUMVAR(*) = VARIANCE OF CUM
C *** FF         = SAMPLE MEAN FOR FIRST PASSAGE
C *** FFVAR     = SAMPLE VARIANCE FOR FIRST PASSAGE
C *** FMBAR(*)  = MEAN OF FREQ
C *** FRCV       = COEFFICIENT OF VARIATION FOR FREQ
C *** FREQ       = NUMBER OF NEW TRANSITIONS INTO ABSORBING STATE
C *** PRVAR(*)  = VARIANCE OF FREQ
C *** I          = DESIRED NUMBER OF MACROREPLICATIONS
C *** INITAL    = INITIAL STATE
C *** ISEDD     = INITIAL SEED
C *** IT          = TRANSITION COUNTER
C *** J          = INDEX FOR STATES
C *** K          = NUMBER OF PARALLEL MICROREPLICATIONS
C *** KPRIME(*) = NUMBER IN STATE AT END OF TRANSITION
C *** KSTAR(*)  = NEXT KPRIME(*)
C *** L          = NUMBER OF DESCRIPTORS TO BE ESTIMATED
C *** LA         = LL + 1
C *** LI         = INDEX FOR I
C *** LIJ        = 1 + OLD
C *** LJ         = INDEX FOR STATES

```

Fig. 1. CHAIN Subroutine

C *** LL	= INDEX FOR L	00000600
C *** LB	= INDEX FOR L	00000610
C *** R(*)	= STATES THAT CAN BE ENTERED FROM J-1	00000620
C *** N	= NUMBER OF HIGHEST STATE	00000630
C *** N1	= NUMBER OF STATES (N+1)	00000640
C *** OLD	= NUMBER OF MACROREPLICATIONS ALREADY PERFORMED (OLD<I)	00000650
C *** OMEGA	= TEST VARIABLE	00000660
C *** P(*)	= TRANSITION MATRIX	00000670
C *** PP	= UQ FROM TIME BEFORE	00000680
C *** PRBAR	= FRACTIONAL PART OF PP	00000690
C *** PSTAR	= INTEGER PART OF PP	00000700
C *** Q(*)	= FROM P	00000710
C *** QQ	= FROM Q AND K	00000720
C *** QBAR	= FRACTIONAL PART OF QQ	00000730
C *** QSTAR	= INTEGER PART OF QQ	00000740
C *** R	= INDEX FOR STATES	00000750
C *** REG	= ACCUMULATED FREQ FOR TRANSITIONS GREATER THAN TT-1	00000760
C *** RPRIME(*)	= CUMULATIVE REWARD FOR ESTIMATORS	00000770
C *** RSEED	= RANDOM GENERATOR SEED, REAL VALUED	00000780
C *** SEED	= RANDOM GENERATOR SEED	00000790
C *** SIZE	= BLOCK SIZE FOR RANDOM NUMBER GENERATOR	00000800
C *** S(J)	= NUMBER OF STATES THAT CAN BE ENTERED FROM J-1	00000810
C *** SJ	= S(J)	00000820
C *** SK	= SUMS(J)	00000830
C *** SS	= MIL (NUMBER OF TRANSITIONS, TT)	00000840
C *** SUMS(J)	= SUM OF S(1) THRU S(J-1), AND SUMS(1)=0	00000850
C *** TT	= MAXIMUM NUMBER OF TRANSITIONS TO LOOK AT	00000860
C *** U	= CURRENT UNIFORM DEVIATE	00000870
C *** V(*)	= UNIFORM DEVIATE ARRAY	00000880
C *** X	= NUMBER OF TRANSITIONS IN CURRENT MOVE	00000890
C *** XBAR(*)	= MEAN MATRIX	00000900
C *** INITIALIZE VARIABLES.		
	PP = 0.000	00000910
	PPVAR = 0.000	00000920
	SS = 0	00000930
	ISEED = SEED	00000940
	RSEED = SEED	00000950
	COUNT = SIZE	00000960
	DO 80 J=1,TT	00000970
	PRVAR(J) = 0.000	00000980
	PRBAR(J) = 0.000	00000990
	CUMVAR(J) = 0.000	00001000
	CUMBAR(J) = 0.000	00001010
80	DO 100 J=1,NP	00001020
	SK = SUMS(J)	00001030
	Q(SK+1) = P(SK+1)	00001040
	IF (S(J).LT.2) GO TO 100	00001050
	SJ = S(J)	00001060
		00001070
		00001080
		00001090

Fig. 1 (Continued)

```

      DO 90 R=2,SJ          00001100
90      Q(SK+R) = Q(SK+R-1)+P(SK+R) 00001110
      W(SK+SJ) = 1.0000D0 00001120
100      CONTINUE 00001130
C *** CHECK IF XBAR AND COV ARE RESTORED. 00001140
      IF (OLD.GT.0) GO TO 115 00001150
      DO 110 LL=1,L 00001160
        XBAR(LL) = 0.0D0 00001170
        COEFF(LL) = 0.0D0 00001180
        DO 110 LM=1,L 00001190
          COV(LL,LM) = 0.0D0 00001200
115      LIJ = 1 + OLD 00001210
      DO 118 LL=1,L 00001220
        XBAR(LL) = XBAR(LL)*OLD 00001230
        DO 118 LM=1,L 00001240
          COV(LL,LM) = COV(LL,LM)*OLD 00001250
118
C *** START MAIN LCCP. 00001260
      DO 540 LI=LIJ,1 00001270
C *** INITIALIZE VARIABLES FOR THIS REPLICATION. 00001280
      B = 0 00001290
      C = (LI-1.0D0)/LI 00001300
      CL = (LI-OLD-1.0D0)/(LI-OLD) 00001310
      CUM = 0.0D0 00001320
      REG = 0.0D0 00001330
      IT = 1 00001340
      OMEGA = 0 00001350
      DO 120 LL=1,L 00001360
        RPRIIME(LL) = 0.0D0 00001370
120      DO 130 J=1,NP 00001380
        KSTAR(J) = 0 00001390
      130      KPRIIME(J) = 0 00001400
C *** START THIS REPLICATION WITH ALL MICROREPLICATIONS IN INITIAL STATE 00001410
      J = INITIAL + 1 00001420
      KPRIIME(J) = K 00001430
      KSTAR(J) = K 00001440
C *** LOOK AT INITIAL STATE. 00001450
      J = INITIAL + 1 00001460
      GO TO 400 00001470
C *** LOOK AT THE NEXT STATE. 00001480
300      J = J+1 00001490
C *** SKIP THE ABSORBING STATE. 00001500
      IF (J.EQ.ABSORB+1) J = J+1 00001510
C *** IF NONE IN THIS STATE, LOOK AT THE NEXT STATE. 00001520
400      IF (KPRIIME(J).EQ.0) GO TO 300 00001530
C *** FIND THE NUMBER OF STATES THAT CAN BE ENTERED FROM STATE J-1. 00001540
      SJ = S(J) 00001550
C *** START WITH THE FIRST STATE THAT CAN BE ENTERED FROM STATE J-1. 00001560
      K = 1 00001570
C *** POINT TO THE NEXT DEVIATE TO USE. 00001580
      00001590

```

Fig. 1 (Continued)

```

COUNT = COUNT + 1                                00001600
C *** GET NEW ARRAY OF DEVIATES IF NEEDED.      00001610
    IF (COUNT.LE.SIZE) GO TO 420                 00001620
    COUNT = 1                                     00001630
C *** CALL RANDOM(SEED,V,SIZE)                  00001640
    CALL GGUBS(RSEED,SIZE,V)                      00001650
C *** GET THE DEVIATE POINTED TO BY COUNT.      00001660
C *** TRANSFORM DEVIATE.                         00001670
420      U          = DBLE(ANOD(KPRIME(J)*V(COUNT),1-)) 00001680
C      WRITE(3,2040) U,V(COUNT)                   00001690
C *** TRANSFER ALL OUT OF THIS STATE FOR TRANSITIONS. 00001700
    KSTAR(J) = KSTAR(J) - KPRIME(J)                00001710
C *** INITIALIZE QQ, QSTAR, AND QBAR.            00001720
    QQ      = 0.0                                    00001730
    QSTAR   = 0                                     00001740
    QBAR    = 0.0                                    00001750
C *** SAVE THE LAST OCCURRENCE OF QQ, QSTAR, AND QBAR. 00001760
500      PP      = UU                           00001770
    PSTAR   = QSTAR                         00001780
    PBAR    = QBAR                          00001790
C *** COMPUTE NEW VALUES FOR QQ, QSTAR, AND QBAR. 00001800
    QQ      = KPRIME(J)*W(SUMS(J)+R)              00001810
    QSTAR   = IDINT(.0)                         00001820
    QBAR    = DMOD(QQ,1.0D0)                     00001830
C *** FIND THE # OF TRANSITIONS TO THE R-TH STATE THAT CAN BE ENTERED. 00001840
C *** FROM J-1.                                 00001850
    X      = (LSTAR-PSTAR)+5*(DSIGN(1.0D0,U-PBAR)+ 00001860
           DSIGN(1.0D0,QBAR-U))                  00001870
C *** ADD THESE TRANSITIONS TO THE ENTERED STATE OCCUPANCY VECTOR. 00001880
    KSTAR(M(SUMS(J)+R)+1) = KSTAR(M(SUMS(J)+R)+1)+X 00001890
C *** FIND THE NUMBER OF TRANSITIONS MADE SO FAR FOR THIS STATE. 00001900
    B      = B+X                               00001910
C *** ACCUMULATE THE REWARDS FOR THIS STATE TRANSITION. 00001920
    DO 510 LL=1,L
        IF (A(LL*(LL-1)+SUMS(J)+R).EQ.0.0.OR.X.EQ.0) GO TO 510 00001930
        RPRIME(LL) = RPRIME(LL)+A(LL*(LL-1)+SUMS(J)+R)*X 00001940
510      CONTINUE                            00001950
C *** GO TO THE NEXT STATE THAT CAN BE REACHED FROM J-1. 00001960
    L      = R+1                               00001970
C *** IF NOT ALL TRANSITIONS WERE MADE FOR THIS STATE, TRY AGAIN. 00001980
    IF (B.LT.KPRIME(J)) GO TO 500               00001990
C *** ACCUMULATE THE NUMBER OF TRANSITIONS MADE SO FAR FOR ALL STATES. 00002000
    OMEGA = OMEGA+B                         00002010
C *** CLEAR THE NUMBER OF TRANSITIONS FOR THE STATE COUNTER. 00002020
    B      = 0                               00002030
C *** IF NOT ALL TRANSITIONS WERE MADE YET, TRY AGAIN. 00002040
    IF (OMEGA.LT.K-KPRIME(ABSORB+1)) GO TO 300 00002050
    OMEGA = 0                               00002060
C *** ACCUMULATE FBAR, FVAR, CUMBAR AND CUMVAR. 00002070
    FREQ = KSTAR(ABSORB+1)-KPRIME(ABSORB+1) 00002080
                                                00002090

```

Fig. 1 (Continued)

```

IF (IT.EQ.1) FREQ = KSTAR(ABSOHB+1)          00002100
FF        = FF + IT*FREQ                      00002110
FFVAR    = FFVAR + IT**2*FREQ                00002120
CUM     = CUM + FREQ                         00002130
LL      = MINO(TT,IT)                        00002140
IF (IT.LT.TT) GO TO 515                      00002150
REG     = REG + FREQ                         00002160
IF (KSTAR(ABSOHB+1).LT.K) GO TO 522          00002170
FREQ = REG                                00002180
515    PRBAR(LL) = PRBAR(LL) + FREQ          00002190
CUMBAR(LL) = CUMBAR(LL) + CUM              00002200
PRVAR(LL) = PRVAR(LL) + FREQ**2            00002210
CUMVAR(LL) = CUMVAR(LL) + CUM**2           00002220
C *** RESET THE STATE OCCUPANCY VECTOR.       00002230
522    DO 525 LJ=1,NP                      00002240
      KPRIME(LJ) = KSTAR(LJ)                  00002250
      SJ = S(LJ)                            00002260
      DO 525 B=1,SJ                      00002270
      KPRIME(B(SUNS(LJ)+B)+1) = KSTAR(B(SUNS(LJ)+B)+1) 00002280
C *** START NEXT TRANSITION IN STATE 0.      00002290
      J = 0                                00002300
C *** COMPUTE THE NUMBER OF TRANSITIONS MADE SO FAR.
      IT = IT + 1                          00002310
C *** IF NOT ALL ABSORBED, TRY AGAIN.
      IF (KPRIME(ABSOHB+1).LT.K) GO TO 300      00002320
C *** RECURSIVE COMPUTATIONS.
      IF (LL.GE.TT) GO TO 529                  00002330
C *** ACCUMULATE CUMBAR AND CUMVAR FOR # OF TRANSITION STEPS > TT-1.
      LL = LL + 1                          00002340
      DO 527 LM=LL,TT                      00002350
        CUMVAR(LM) = CUMVAR(LM) + CUM**2
      527   CUMBAR(LM) = CUMBAR(LM) + CUM          00002360
C *** COMPUTE THE COVARIANCE MATRIX RECURSIVELY.
      529   IF (LI.EQ.1) GO TO 535                  00002370
      DO 530 LI=1,L
        DO 530 LM=1,L
          COV(LL,LM) = ((LI-2)*COV(LL,LM)+(RPRIME(LL)/K-XBAR(LL))* 00002380
          1          (RPRIME(LM)/K-XBAR(LM))*C)/(LI-1)          00002390
C *** COMPUTE SS.
      535   SS = MINO(TT,MAX0(SS,IT-1))          00002400
C *** COMPUTE THE SAMPLE MEAN VECTOR RECURSIVELY.
      DO 540 LI=1,L
        XBAR(LL) = C*XBAR(LL)+(1.0D0-C)*RPRIME(LL)/K      00002410
      540   CONTINUE                           00002420
C *** END MAIN LOOP, COMPLETED I MACROREPLICATIONS.
C ***
C *** COMPUTE PRBAR, PRVAR, CUMBAR, AND CUMVAR DIRECTLY.
      IF (I.NE.1) BEG = (K**2.0D0)*(I**2.0D0)*(I-1.0D0) 00002430
      DO 545 LL=1,TT                          00002440
                                              00002450
                                              00002460
                                              00002470
                                              00002480
                                              00002490
                                              00002500
                                              00002510
                                              00002520
                                              00002530
                                              00002540
                                              00002550
                                              00002560
                                              00002570
                                              00002580
                                              00002590

```

Fig. 1 (Continued)

```

      IF (I.EQ.1) GO TO 544          00002600
      PRVAR(LL) = (I*PRVAR(LL)-PRBAR(LL)**2)/REG 00002610
      CURVAR(LL) = (I*CURVAR(LL)-CURBAR(LL)**2)/REG 00002620
544      CUMBAR(LL) = CUMBAR(LL)/(K*I) 00002630
545      PRBAR(LL) = PRBAR(LL)/(K*I) 00002640
                                00002650
      DO 550 LL=1,L                00002660
      DO 550 LM=1,L                00002670
550      COV(LL,LM) = COV(LL,LM)/L 00002680
      DO 570 LL=1,L                00002690
      IF (XBAR(LL).NE.0) COEFF(LL) = DSQRT(COV(LL,LL))/KBAR(LL) 00002700
      IF (LL.EQ.1) GO TO 570 00002710
      LA = LL+1 00002720
      DO 560 LM=LA,L 00002730
      IF (COV(LL,LL)*COV(LM,LM).GT.0) 00002740
1       COV(LM,LL)=COV(LL,LM)/DSQRT(COV(LL,LL)*COV(LM,LM)) 00002750
560      CONTINUE 00002760
570      CONTINUE 00002770
                                00002780
C *** PRINT RESULTS.          00002790
                                00002800
      SEED = MSEED 00002810
      WRITE (3,1000) NP,INITIAL,ABSORB,ALL,L,K,I,ISEED,SEED,SIZE 00002820
1000  FORMAT(1H1,*RESULTS OF ROTATION SAMPLING FOR A MARKOV CHAIN*////. 00002830
      1* NO. OF STATES          =*,I10//, 00002840
      2* INITIAL STATE          =*,I10//, 00002850
      3* ABSORBING STATE        =*,I10//, 00002860
      4* TOTAL NO. OF (I,J) PAIRS =*,I10//, 00002870
      5* NO. OF DESCRIPTORS     =*,I10//, 00002880
      6* NO. OF CORRELATED MICROREPLICATIONS =*,I10//, 00002890
      7* NO. OF INDEPENDENT MACROREPLICATIONS =*,I10//, 00002900
      8* INITIAL SEED           =*,I10//, 00002910
      9* FINAL SEED             =*,I10//, 00002920
      C* BLOCKING FACTOR       =*,I10//, 00002930
      REWIND 11 00002940
      WRITE (3,2000) 00002950
      WRITE (3,2030) 00002960
      WRITE (3,2040) (XBAR(LL),LL=1,L) 00002970
      WRITE (3,2010) 00002980
      WRITE (3,2030) 00002990
      WRITE (3,2040) (COEFF(LL),LL=1,L) 00003000
      WRITE (3,2020) 00003010
      WRITE (3,2030) 00003020
      DO 580 LL=1,L 00003030
      WRITE (3,2045) LL,(COV(LL,LM),LM=1,L) 00003040
580      CONTINUE 00003050
2000  FORMAT(//,* SAMPLE MEAN VECTOR*//, 00003060
1       * ***** *//, 00003070
2010  FORMAT(//,* SAMPLE COEFFICIENTS OF VARIATION*//, 00003080
1       * ***** *//, 00003090

```

Fig. 1 (Continued)

```

2020 FORMAT(//,' SAMPLE COVARIANCE/CORRELATION MATRIX',//,
1      ' .....ooooooooooooooo.....',//)
2030 FORMAT(9X,'1',14X,'2',14X,'3',14X,'4',14X,'5',14X,'6',14X,'7',
1      '14X,'8',14X,'9',//)
2040 FORMAT(2X,9(D15.8)//)
2045 FORMAT(12,9(D15.8)//)
    FF      = FF/(K*I)
    FFVAR   = FFVAR/(K*I) - FF**2
    DO 620 LL=1,SS
        PRCV = 0.0
        CUMCV = 0.0
        IF (PRBAR(LL).NE.0.0D0) PRCV=DSQRT(PRVAR(LL))/PRBAR(LL)
        IF (CUMBAR(LL).NE.0.0D0) CUMCV=DSQRT(CUMVAR(LL))/CUMBAR(LL)
        IF (MOD(LL,50).NE.1) GO TO 620
        WRITE (3,3000)
        IF (LL.GT.1) GO TO 610
        WRITE (3,3010) FF,FFVAR
610      WRITE (3,3020)
620      WRITE (3,3030) LL,PRBAR(LL),PRVAR(LL),PRCV,CUMBAR(LL),
1                      CUMVAR(LL),CUMCV
        IF (OLD.EQ.0) RETURN
        LL = I - OLD
        WRITE (3,4000) LL
3000 FORMAT(141,'FIRST PASSAGE TIME (T) DISTRIBUTION',//,
1      ' .....ooooooooooooooo.....')
3010 FORMAT(/,1X,'SAMPLE MEAN(T) =',D15.8,5X,
1      'SAMPLE VARIANCE(T) =',D15.8)
3020 FORMAT(/,33X,'MASS FUNCTION',42X,'DISTRIBUTION FUNCTION',//,
1      '35X,'VARIANCE',10X,'COEFFICIENT',
2      '31X,'VARIANCE',10X,'COEFFICIENT',//,
3      '  1',10X,'PB(T=I)',11X,'OF PR(T=I)',9X,'OF VARIATION',
4      '  10X,'PR(T<=I)',10X,'OF PB(T<=I)',9X,'OF VARIATION',
5      '/'  ' ---',9X,'-----',11X,'-----',9X,'-----',
6      '  10X,'-----',10X,'-----',9X,'-----')
3030 FORMAT(' ',15.6(5X,D15.8))
4000 FORMAT(/,' FIRST PASSAGE DISTRIBUTION IS BASED ON THE LAST ',
1      ' 15.' MACROREPLICATIONS.')
    RETURN
    END

```

Fig. 1 (Continued)

Fig. 2 Input to CHAIN Subprogram

(a) Data Input

VARIABLE	TYPE	DESCRIPTION
A	REAL*4(ASIZE)	$A(ALL*(LL-1) + SUMS(J) + R) = \text{reward received when a replication jumps from state } J - 1 \text{ to state } M(SUMS(J) + R) \text{ for } R = 1, \dots, S(J) \text{ for reward function } LL = 1, 2, \dots, L$
ABSORB	INTEGER	Absorbing state $0 \leq \text{ABSORB} \leq N + 1$
ALL	INTEGER	Total number of arcs = $SUMS(NP) + S(NP)$
ASIZE	INTEGER	ALL*L
I	INTEGER	Desired number of independent macroreplications
INITAL	INTEGER	Initial state $0 \leq \text{INITAL} \leq N + 1$
K	INTEGER	Number of parallel microreplications per macroreplication
L	INTEGER	Total number of reward functions
M	INTEGER(N+1)	$M(SUM(J) + LR) = LR\text{th of } S(J) \text{ states to which a replication can move from state } J - 1$ $LR = 1, \dots, S(J)$
NP	INTEGER	$NP = N + 1 = \text{total number of states}$
OLD	INTEGER	If $OLD = 0$ simulation proceeds to run I macroreplications If $OLD > 0$ simulation proceeds to run $I - OLD$ additional macroreplications
P	REAL*4(ALL)	$P(SUM(J) + LR) = \text{probability of moving from state } J - 1 \text{ to } M(SUM(J) + LR) \text{ } LR = 1, \dots, S(J)$
S	INTEGER(N+1)	$S(J) = \text{number of states that can be entered from state } J - 1$
SEED	INTEGER	Initial value for random number generator
SIZE	INTEGER	Each call to the random number generator returns a block of SIZE uniform deviates

(continued)

Fig. 2 (Continued)

(a)

VARIABLE	TYPE	DESCRIPTION
SUMS	INTEGER(NP)	$\text{SUMS}(J) = 0 \quad J = 1$ $= \sum_{I=1}^{J-1} S(I) \quad J = 2, \dots, NP$
TT	INTEGER	Number of cells in sample first passage time distribution. Last cell estimates probability of absorption at time $\geq TT$

(b) Working Arrays

VARIABLE	TYPE	DESCRIPTION
KPRIME	INTEGER(NP)	Distribution of microreplications by state at end of a transition
KSTAR	INTEGER(NP)	Distribution of microreplications by state at beginning of a transition
Q	REAL*8(ALL)	$Q(\text{SUM}(J) + LR) = \text{probability of moving from state } J - 1 \text{ to state } M(\text{SUM}(J) + 1), M(\text{SUM}(J) + 2), \dots \text{ or } M(\text{SUM}(J) + LR)$ $LR = 1, \dots, S(J)$
RPRIME	REAL*8(L)	Accumulated rewards for L reward functions
V	REAL*4(SIZE)	Space to store uniform deviates

(continued)

Fig. 2 (Continued)

(c) Arrays Used to Summarize Data on I Macroreplications

VARIABLE	TYPE	DESCRIPTION
COEFF	REAL*8(L)	COEFF(J1) = sample coefficient of variation of XBAR(J1) J1=1,...,L
COV	REAL*8(L,L)	At completion COV(J1, J2) contains the sample covariance of XBAR(J1) and XBAR(J2) for J2=J1,...,L and J1=1,...,L and COV(J2,J1) contains the sample correlation between XBAR(J1) and XBAR(J2) for J1=1,...,J2-1 and J2=2,...,L .
CUMBAR	REAL*8(TT)	CUMBAR(J1) = sample probability that absorption occurs on a step \leq J1 for J1=1,...,TT - 1; CUMBAR(TT) = 1
CUMVAR	REAL*8(TT)	CUMVAR(J1) = Sample variance of CUMBAR(J1) J1=1,...,TT
FF	REAL*8	Sample mean of first passage time.
FFVAR	REAL*8	Sample variance of first passage time.
FRBAR	REAL*8(TT)	FRBAR(J1) = sample absorption probability at step J1 for J1=1,...,TT - 1 $FRBAR(TT) = 1 - \sum_{J1=1}^{TT-1} FRBAR(J1)$
FRVAR	REAL*8(TT)	FRVAR(J1) = sample variance of FRBAR(J1) J1=1,...,TT
XBAR	REAL*8(L)	XBAR(J1) = the sample mean reward for reward function J1=1,...,L

```

INTEGER I,J,KPBINE(50),KSTAR(50),L,K,LL,N(100),N,NP,S(50).          00000100
1      SUMS(50),ALL,INITAL,ABSORB,SIZE,OLD,SEED,TT,ASIZE           00000110
REAL*4  A(500),LAM,V(40000),W           00000120
REAL*8  COEPP(10),COV(10,10),U(100),PRIME(10),YBAR(10).          00000130
1      P(100),PRVAR(100),PRBAR(100),CUMBAR(100),CUMVAR(100)        00000140
00000150
C *** INITIALIZE VALUES.                                         00000160
00000170
      READ (1,1000) N,L,K,LAM,W,I,ABSORB,INITAL,SIZE,TT           00000180
1000  FORMAT (15.,/13.,/16.,/F4.1./,F4.1./,15.,/15.,/15.,/15.)    00000190
      WRITE(3,1005) N,L,K,LAM,W,I,ABSORB,INITAL,SIZE,TT           00000200
1005  FORMAT (' N=',15.,' L=',13.,' K=',16.,'          00000210
1      ' LAM=',F4.1.,' W=',F4.1.,' I=',15.,' ABSORB=',15.,          00000220
2      ' INITAL=',15.,' SIZE=',15.,' TT=',15.)                   00000230
00000240
      NP = N + 1                                         00000250
      READ (11,1020) SEED                           00000260
1020  FORMAT(I10)
C *** FOR EACH STATE DETERMINE THE NUMBER OF STATES THAT CAN BE ENTERED. 00000270
      S(1) = 1                                         00000280
      DO 80 J=2,NP                                     00000290
80      S(J) = 2                                         00000300
      WRITE(3,1015) (S(J),J=1,NP)                      00000310
1015  FORMAT (' S(J)      =',20I5)                  00000320
      SUMS(1) = 0                                         00000330
      ALL = S(1)                                         00000340
      DO 90 J=2,NP                                     00000350
90      SUMS(J) = ALL                                00000360
      ALL = ALL + S(J)                               00000370
C *** THE NEXT INITIALIZATIONS MAY BE RUN SPECIFIC.          00000380
      OLD = 0                                         00000390
      DO 100 J=2,NP                                     00000400
100    COMPUTE TRANSITION PROBABILITIES.                 00000410
      P(SUMS(J)+1) = N/(LAM+W)                         00000420
      P(SUMS(J)+2) = LAM/(LAM+W)                        00000430
      CONTINUE                                         00000440
      P(1) = 1.0                                         00000450
      WRITE (3,1016) (P(LL),LL=1,ALL)                  00000460
1016  FORMAT (' P(*)      =',20F5.2)                00000470
C *** FOR EACH STATE J DETERMINE STATES THAT CAN BE ENTERED. 00000480
      DO 400 J=2,N                                         00000490
400    M(SUMS(J)+1) = J-2                            00000500
      M(SUMS(J)+2) = J                                00000510
      M(1) = 1                                         00000520
      M(SUMS(NP)+1) = N-1                            00000530
      M(SUMS(NP)+2) = N                            00000540
      WRITE (3,1017) (M(LL),LL=1,ALL)                  00000550
1017  FORMAT (' M(*)      =',20I5)                00000560
C *** COMPUTE REVERSE VECTOR.                          00000570
      DO 500 J=1,NP                                     00000580
      A(ALL+2+SUMS(J)+1) = 0.0                         00000590

```

Fig. 3 Driver Routine for Example

```
A(ALL+2+SUMS(J)+2) = 0.0          00000600
A(ALL+3+SUMS(J)+1) = 0.0          00000610
A(ALL+3+SUMS(J)+2) = 0.0          00000620
A(SUMS(J)+1)           = N(SUMS(J)+1)/(LAH+N) 00000630
A(SUMS(J)+2)           = N(SUMS(J)+2)/(LAH+N) 00000640
A(ALL+SUMS(J)+1)       = 1/(LAH+N)            00000650
500   A(ALL+SUMS(J)+2)       = 1/(LAH+N)            00000660
      A(ALL+SUMS(2)+1)       = 1/LAH              00000670
      A(ALL+2+1)             = 1/(LAH+N)            00000680
      A(ALL+2+SUMS(3)+1)     = 1/(LAH+N)            00000690
      A(ALL+3+SUMS(2)+2)     = 1/(LAH+N)            00000700
      A(ALL+3+SUMS(4)+1)     = 1/(LAH+N)            00000710
DO 550 LL=1,L
      WRITE(3,1018) (A(ALL+(LL-1)+LR), LR=1, ALL) 00000720
1018 FORMAT (' A(*,LL)  *', 20F5.2)
550   CONTINUE
      ASIZE = ALL*L
      C *** CALL PARALLEL SIMULATION PROGRAM.
      CALL CHAIN(K,GLD,I,NP,INITIAL,ABSORB,S,N,SUMS,ALL,P,KPRIME,
1          KSTAR,Q,L,ASIZE,A,PRIME,XBAR,COV,COEFF,TT,PRBAR,
2          PRVAR,CUMBAR,CURVAR,SEED,SIZE,V)
      STOP
      END
```

Fig. 3 (Continued)

Fig. 4 Sample Output from CHAIN Subroutine

RESULTS OF ROTATION SAMPLING FOR A NARROW CHAIN

NO. OF STATES	-	50
INITIAL STATE	-	0
ABSORBING STATE	-	0
TOTAL NO. OF (I,J) PAIRS	-	99
NO. OF DESCRIPTORS	-	4
NO. OF COORDINATE ALGORITHMS	-	131072
NO. OF INDEPENDENT ALGORITHMS	-	4
INITIAL SEED	-	1234567
FINAL SEED	-	590573803
BLOCKING FACTOR	-	40000

SAMPLE STATE VECTORS

1	2	3	4	5	6	7	8	9
0.9653361e-02	0.1105240e02	0.999963559	00	0.8998891580	00			

SAMPLE COEFFICIENTS OF VARIATION

1	2	3	4	5	6	7	8	9
0.25163951e-02	0.70220364e-03	0.59198837e-04	0.13659310e-03					

SAMPLE COVARIANCE/CORRELATION MATRIX

1	2	3	4	5	6	7	8	9
0.5908196e-01	0.17939022e-02	0.-37050189e-05	0.-57659548e-05					
0.9508246e00	0.60247435e-04	0.19277545e-06	0.-34303695e-06					
0.-2577712e00	0.4195513e00	0.350e2466e-08	0.-7071316e0-08					
0.1929856e00	0.35954652e00	0.971815e10	0.15109075e-07					

Fig. 4 (Continued)

FIRST PASSAGE TIME (T) DISTRIBUTION

SAMPLE MEAN(\bar{x}) = 0.198869850 02 SAMPLE VARIANCE (s^2) = 0.640114330 04

I	$P(T < t)$	BASES FUNCTION		COEFFICIENT OF VARIATION OF $P(T < t)$	DISTRIBUTION FUNCTIONS
		VARIANCE OF $P(T < t)$	$P(T < t)$		
1	0.0	0.0	0.265246405-05	0.526316640 00	0.0 0.265246405-05
2	0.526316640 00	0.194891720-11	0.526316640 00	0.194891720-11	0.0 0.265246405-05
3	0.0	0.0	0.526316640 00	0.194891720-11	0.0 0.265246405-05
4	0.131212230 00	0.155913380-11	0.951628328-05	0.657528880 00	0.402776230-11 0.305222875-05
5	0.0	0.0	0.657528880 00	0.657528880 00	0.0 0.305222875-05
6	0.654268260-01	0.194891720-11	0.2133373572-04	0.722955700 00	0.155913380-11 0.172714950-05
7	0.0	0.0	0.722955700 00	0.722955700 00	0.0 0.172714950-05
8	0.807781600-01	0.298833970-11	0.423923348-04	0.763733860 00	0.506718480-11 0.294741490-05
9	0.0	0.0	0.763733860 00	0.763733860 00	0.0 0.294741490-05
10	0.284662250-01	0.506718480-11	0.790775962-04	0.792200990 00	0.363797980-11 0.240765980-05
11	0.0	0.0	0.792200990 00	0.792200990 00	0.0 0.240765980-05
12	0.2129077390-01	0.194891720-11	0.655699842-04	0.813490870 00	0.298833970-11 0.212501620-05
13	0.0	0.0	0.813490870 00	0.813490870 00	0.0 0.212501620-05
14	0.166784100-01	0.298833970-11	0.103645362-03	0.830169680 00	0.623653510-11 0.300818650-05
15	0.0	0.0	0.830169680 00	0.830169680 00	0.0 0.300818650-05
16	0.1351811330-01	0.298833970-11	0.127876828-03	0.843688010 00	0.298833970-11 0.204895790-05
17	0.0	0.0	0.843688010 00	0.843688010 00	0.0 0.204895790-05
18	0.112304690-01	0.207884500-11	0.1283884678-03	0.854918480 00	0.506718480-11 0.263304720-05
19	0.0	0.0	0.854918480 00	0.854918480 00	0.0 0.263304720-05
20	0.952243860-02	0.909494700-12	0.100150220-03	0.864440920 00	0.931538010-11 0.313588380-05
21	0.0	0.0	0.864440920 00	0.864440920 00	0.0 0.313588380-05
22	0.81996180-02	0.155913380-11	0.152280452-03	0.872640610 00	0.779566890-11 0.319956690-05
23	0.0	0.0	0.872640610 00	0.872640610 00	0.0 0.319956690-05
24	0.715253740-02	0.207884500-11	0.201581050-03	0.879793170 00	0.779566890-11 0.317355330-05
25	0.0	0.0	0.879793170 00	0.879793170 00	0.0 0.317355330-05
26	0.631237030-02	0.402776230-11	0.317935602-03	0.886105540 00	0.185796770-10 0.486444790-05
27	0.0	0.0	0.886105540 00	0.886105540 00	0.0 0.486444790-05
28	0.562900270-02	0.194891720-11	0.248808690-03	0.891725540 00	0.181898940-10 0.476281800-05
29	0.0	0.0	0.891725540 00	0.891725540 00	0.0 0.476281800-05
30	0.50439350-02	0.909494700-12	0.189071650-03	0.896769520 00	0.165008320-10 0.452972740-05
31	0.0	0.0	0.896769520 00	0.896769520 00	0.0 0.452972740-05
32	0.455856320-02	0.207884500-11	0.316288090-03	0.901328090 00	0.13325650-10 0.405869830-05
33	0.0	0.0	0.901328090 00	0.901328090 00	0.0 0.405869830-05
34	0.414657590-02	0.207884500-11	0.347713240-03	0.905474660 00	0.227373680-10 0.526615620-05
35	0.0	0.0	0.905474660 00	0.905474660 00	0.0 0.526615620-05
36	0.378793440-02	0.207884500-11	0.380628710-03	0.909262660 00	0.175402550-10 0.460604860-05
37	0.0	0.0	0.909262660 00	0.909262660 00	0.0 0.460604860-05
38	0.347900390-02	0.207884500-11	0.414434590-03	0.912741660 00	0.175402550-10 0.458849260-05
39	0.0	0.0	0.912741660 00	0.912741660 00	0.0 0.458849260-05
40	0.872583390-01	0.175402550-10	0.479966550-04	0.100000000 01	0.0 0.0

Fig. 4. (Continued)

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20. presents applications of interest for first passage time and steady-state distributions in Section 2. Section 3 describes the algorithm and CHAIN and an example in Section 4 illustrates how CHAIN works in practice. Section 5 describes the options available for restarting the simulation.

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